Research Article

The Global Cyclicity Index of Benzenoid Chains

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The resistance distance $\Omega_G(i, j)$ between vertices i and j of a connected (molecular) graph G is computed as the effective resistance between nodes i and j in the corresponding network constructed from G by replacing each edge of G with a unit resistor. The conductance excess between any i and j of G is the difference between $1/\Omega_G(i, j)$ and the reciprocal of the distance between i and j . The global cyclicity index of G is defined as the sum of conductance excesses between all pairs of adjacent vertices. In this paper, by computing resistance distances between pairs of adjacent vertices in linear polyacenes, an explicit formula for the global cyclicity index of a benzenoid chain is obtained in terms of its number of hexagons.

1. Introduction

As the number of possible chemical compounds is so big, their huge part will never be experimentally tested. For this reason, there is a need for mathematical modeling and analysis of certain classes of compounds. To this end, many topological indices are defined and applied in the modeling of chemical and pharmacological properties of molecules. In the present work, we will take a new molecular cyclicity measure into consideration.

There are different possible measures of “cyclicity” of a molecular graph $G = (V(G), E(G))$. One simple such traditional fundamental measure is the cyclomatic number $\mu(G)$ (also called the first Betti number, the nullity, or the cycle rank) which is defined for a connected graph G with n vertices and m edges as

$$\mu(G) = m - n + 1. \quad (1)$$

Motivated from electrical network theory, Klein and Ivanciuc proposed a new cyclicity measure. This new cyclicity measure is established on the basis of the novel concept of resistance distance [1–7]. As an intrinsic graph metric, the resistance distance $\Omega_G(i, j)$ between vertices i and j of a connected (molecular) graph G is computed as the effective resistance between nodes i and j in the corresponding network constructed from G by replacing each edge of G with a unit

resistor. Comparing to the traditional (shortest path) distance $d_G(i, j)$ between i and j , it is well known that $\Omega_G(i, j)$ equals the length $d_G(i, j)$ of the shortest path between i and j if there is a unique single path between i and j , while if there is more than one path, then $\Omega_G(i, j)$ is strictly less than $d_G(i, j)$. Thence, the conductance excess $\sigma_G(i, j) - 1/d_G(i, j)$ indicates in some manner the presence of cyclicity in the portion of the graph interconnecting i and j , where $\sigma_G(i, j) = 1/\Omega_G(i, j)$ is known as the effective conductance between i and j . To measure the cyclicity of a graph G , Klein and Ivanciuc [8] proposed the global cyclicity index $C(G)$ as

$$C(G) = \sum_{i \sim j} \left[\sigma_G(i, j) - \frac{1}{d_G(i, j)} \right], \quad (2)$$

where $i \sim j$ means that i and j are adjacent and the sum is over all edges of G . Since $d_G(i, j) = 1$ for $i \sim j$, $C(G)$ can also be written as

$$C(G) = \sum_{i \sim j} [\sigma_G(i, j) - 1] = \sum_{i \sim j} \sigma_G(i, j) - |E(G)|. \quad (3)$$

As a new measure of cyclicity of graphs, the global cyclicity index has less degeneracy than the standard cyclomatic number and has some intuitively appealing features. Since the idea of cyclicity is related to measures of connectivity or complexity [9] and characterization of “cyclicity” is an

FIGURE 1: A benzenoid chain with n hexagons (a) and the linear polyacene L_n (b).

aspect of key importance in the study of molecular graphs [10, 11], it is worth studying the global cyclicity index from both mathematical and chemical points of view.

A *benzenoid system* is a 1-connected collection of congruent regular hexagons arranged in the plane in such a way that any two hexagons having a common point intersect in a whole edge. The vertices lying on the border of the unbounded face of a benzenoid system are called external; other vertices, if present, are called internal. A benzenoid system without internal vertices is called *catacondensed*. If no hexagon in a catacondensed benzenoid is adjacent to three other hexagons, we say that the benzenoid is a *benzenoid chain*. If a benzenoid chain has no turn hexagons, then it is called a *linear polyacene*.

In [8], Klein and Ivanciuc established a number of theorems for the global cyclicity index of graphs (even not connected). In [12], one of the present authors obtained bounds for the global cyclicity index of fullerene graphs. In [13], one of the present authors also obtained some further results on the global cyclicity number, including the strictly monotone increasing property, some lower and upper bounds, and some Nordhaus-Gaddum-type results, a relationship between $C(G)$ and the cyclomatic number $\mu(G)$. In this paper, by computing resistance distances between pairs of adjacent vertices in linear polyacenes, an explicit formula for the global cyclicity index of benzenoid chains is obtained in terms of the number of hexagons.

2. Results

2.1. Resistance Distances between Adjacent Vertices in Linear Polyacenes. In this subsection, we will compute resistance distances between pairs of adjacent vertices in linear polyacenes. Denote by L_n the linear polyacene with n hexagons. For convenience, we label the vertices of L_n as depicted in Figure 1.

To compute resistance distances between pairs of adjacent vertices in L_n , we need to employ the classical result of computing resistance distances in terms of spanning trees and spanning bi-trees. A spanning tree (resp., forest) of a connected graph G is a subgraph that contains all the vertices and is a tree (resp., forest). A spanning bi-tree of a connected graph is defined as a spanning forest of the graph with exactly

two components. A spanning bi-tree is said to separate vertices i and j if the vertices i and j are in distinct components of the bi-tree. For a connected graph G and for any two vertices $i, j \in V(G)$, we denote by $t(G)$ and $t(G; i, j)$ the number of spanning trees of G and the number of spanning bi-trees of G separating i and j , respectively. Then resistance distances can be computed as given in the following Lemma.

Lemma 1 (see [14]). *Let G be a connected graph. Then the resistance distance between any two vertices i and j in G can be computed as*

$$\Omega_G(i, j) = \frac{t(G; i, j)}{t(G)}. \quad (4)$$

Now suppose that i and j are adjacent in G , and let e be an edge connecting them. If T is a spanning tree that contains e , then by the deletion of e from T we could obtain a spanning bi-tree F separating i and j . Conversely, if F is a spanning bi-tree separating i and j , then by adding a new edge e connecting i and j to F we could obtain a spanning tree of G . So, the number of spanning trees containing e is equal to the number of spanning bi-trees separating i and j . While, on the other hand, the number of spanning trees of G that contain e is equal to the number of spanning trees of the graph G/e , where G/e denotes the graph obtained from G by contracting e , that is, deleting e and then identifying two end vertices of e . Thus, as a consequence of Lemma 1, we have the following result.

Lemma 2. *Let G be a connected graph with $e = ij \in E(G)$. Then*

$$\Omega_G(i, j) = \frac{t(G/e)}{t(G)}. \quad (5)$$

In the enumeration of spanning trees of graphs, there is a famous recursion formula, known as the deletion-contraction recurrence. As stated in the following lemma, the recursion formula is applicable to *multiple graphs* (i.e., graphs with multiple edges).

Lemma 3. *Let G be a multiple graph, and let e be an edge of G . Then*

$$t(G) = t(G - e) + t\left(\frac{G}{e}\right), \quad (6)$$

where $G - e$ denotes the graph obtained from G by the deletion of e .

Combining Lemmas 2 and 3, we readily have Lemma 4.

Lemma 4. Let G be a connected graph with $e = ij$ being an edge of G . Then

$$\Omega_G(i, j) = \frac{t(G) - t(G - e)}{t(G)}. \quad (7)$$

For computing resistance distances between adjacent vertices in L_n , the number of spanning trees of L_n plays an essential rule.

Lemma 5 (see [15–17]). Consider

$$t(L_n) = \frac{\sqrt{2}}{8} \left[(3 + 2\sqrt{2})^{n+1} - (3 - 2\sqrt{2})^{n+1} \right]. \quad (8)$$

Now we are arriving at Theorem 6.

Theorem 6. Resistance distances between pairs of adjacent vertices of a linear polyacene could be computed as follows.

For $1 \leq k \leq n$,

$$\begin{aligned} \Omega_{L_n}(a_k, b_k) &= \Omega_{L_n}(b_k, a_{k+1}) = \Omega_{L_n}(a'_k, b'_k) = \Omega_{L_n}(b'_k, a'_{k+1}) \\ &= \left(\left[1 - \frac{\sqrt{2}}{8} + \frac{\sqrt{2}}{8} (3 - 2\sqrt{2})^{2k} \right] (3 + 2\sqrt{2})^{n+1} \right. \\ &\quad \left. - \left[1 + \frac{\sqrt{2}}{8} - \frac{\sqrt{2}}{8} (3 + 2\sqrt{2})^{2k} \right] (3 - 2\sqrt{2})^{n+1} \right) \\ &\quad \times \left((3 + 2\sqrt{2})^{n+1} - (3 - 2\sqrt{2})^{n+1} \right)^{-1}, \end{aligned} \quad (9)$$

for $1 \leq k \leq n + 1$,

$$\begin{aligned} \Omega_{L_n}(a_k, a'_k) &= \frac{\sqrt{2}}{2} \left(\left[1 + (3 - 2\sqrt{2})^{2k-1} \right] (3 + 2\sqrt{2})^{n+1} \right. \\ &\quad \left. + \left[1 + (3 + 2\sqrt{2})^{2k-1} \right] (3 - 2\sqrt{2})^{n+1} \right) \\ &\quad \times \left((3 + 2\sqrt{2})^{n+1} - (3 - 2\sqrt{2})^{n+1} \right)^{-1}. \end{aligned} \quad (10)$$

Proof. We first compute resistance distances between adjacent degree two and degree three vertices. For $1 \leq k \leq n$, by the structure of L_n , we could see that

$$\Omega_{L_n}(a_k, b_k) = \Omega_{L_n}(b_k, a_{k+1}) = \Omega_{L_n}(a'_k, b'_k) = \Omega_{L_n}(b'_k, a'_{k+1}). \quad (11)$$

By Lemma 4, we have

$$\Omega_{L_n}(a_k, b_k) = \frac{t(L_n) - t(L_n - a_k b_k)}{t(L_n)}. \quad (12)$$

Notice that the number of spanning trees of the graph $L_n - a_k b_k$ is equal to the product of the number of spanning trees of L_{k-1} and the number of spanning trees of L_{n-k} (here the number of spanning trees of L_0 is regarded as 1, and the formula in Lemma 5 is also applicable to L_0); that is,

$$t(L_n - a_k b_k) = t(L_{k-1}) t(L_{n-k}). \quad (13)$$

Hence,

$$\Omega_{L_n}(a_k, b_k) = \frac{t(L_n) - t(L_{k-1}) t(L_{n-k})}{t(L_n)}. \quad (14)$$

Substituting (8) into the above equality, we could obtain (9). It should be mentioned that to obtain (9), one should notice that $3 + 2\sqrt{2}$ is the reciprocal of $3 - 2\sqrt{2}$.

Now, we compute resistance distances between $\{a_k, a'_k\}$ ($1 \leq k \leq n + 1$). Denote by S_n the graph obtained from L_n by contracting the edge $a_1 b_1$; that is, $S_n = L_n / a_1 b_1$. Noticing that the number of spanning trees of $L_n - a_1 b_1$ is equal to the number of spanning trees of L_{n-1} , by Lemma 3, simple calculation leads to

$$\begin{aligned} t(S_n) &= t(L_n) - t(L_n - a_1 b_1) = t(L_n) - t(L_{n-1}) \\ &= \frac{\sqrt{2}}{4} \left[(\sqrt{2} + 1)^{2n+1} + (\sqrt{2} - 1)^{2n+1} \right]. \end{aligned} \quad (15)$$

If we regard the number of spanning trees of S_0 as 1, then (15) also holds for $n = 0$. Let $L_n / a_k a'_k$ be the graph obtained from L_n by contracting the edge $a_k a'_k$. Then it is not hard to observe that

$$t\left(\frac{L_n}{a_k a'_k}\right) = t(S_{k-1}) t(S_{n-k+1}). \quad (16)$$

Hence, by Lemma 2, for $1 \leq k \leq n + 1$,

$$\Omega_{L_n}(a_k, a'_k) = \frac{t(L_n / a_k a'_k)}{t(L_n)} = \frac{t(S_{k-1}) t(S_{n-k+1})}{t(L_n)}. \quad (17)$$

Substituting (8) and (15) into the above equality, we could obtain (10). $\square$

2.2. The Global Cyclicity Index of Benzenoid Chains. In [8], Klein and Ivanciuc obtained the following result in Lemma 7.

Lemma 7 (see [8]). All benzenoid chains with the same number of hexagons have the same global cyclicity index.

Now we are ready to give the main result of the paper.

TABLE 1

G	$Kf(G)$	G	$Kf(G)$	G	$Kf(G)$	G	$Kf(G)$	G	$Kf(G)$
H_1	1.2	H_{11}	13.927	H_{21}	26.669	H_{31}	39.39	H_{41}	52.122
H_2	2.469	H_{12}	15.2	H_{22}	27.932	H_{32}	40.664	H_{42}	53.395
H_3	3.7419	H_{13}	16.474	H_{23}	29.205	H_{33}	41.937	H_{43}	54.668
H_4	5.0151	H_{14}	17.747	H_{24}	30.478	H_{34}	43.21	H_{44}	55.942
H_5	6.2883	H_{15}	19.02	H_{25}	31.752	H_{35}	44.483	H_{45}	57.215
H_6	7.5614	H_{16}	20.293	H_{26}	33.025	H_{36}	45.756	H_{46}	58.488
H_7	8.8346	H_{17}	21.566	H_{27}	34.298	H_{37}	47.029	H_{47}	59.761
H_8	10.108	H_{18}	22.839	H_{28}	35.571	H_{38}	48.303	H_{48}	61.034
H_9	11.318	H_{19}	24.113	H_{29}	36.844	H_{39}	49.576	H_{49}	62.307
H_{10}	12.654	H_{20}	25.386	H_{30}	38.117	H_{40}	50.849	H_{50}	63.581

Theorem 8. Let H_n be a benzenoid chain with n hexagons. Then

$$\begin{aligned}
C(H_n) = & 4 \sum_{k=1}^n \left(\left[1 - (3 - 2\sqrt{2})^{2k} \right] (3 + 2\sqrt{2})^{n+1} \right. \\
& + \left[1 + (3 + 2\sqrt{2})^{2k} \right] (3 - 2\sqrt{2})^{n+1} \Big) \\
& \times \left(\left[4\sqrt{2} - 1 + (3 - 2\sqrt{2})^{2k} \right] (3 + 2\sqrt{2})^{n+1} \right. \\
& - \left[4\sqrt{2} + 1 - (3 + 2\sqrt{2})^{2k} \right] (3 - 2\sqrt{2})^{n+1} \Big)^{-1} \\
& + \sum_{k=1}^{n+1} \left(\left[\sqrt{2} - 1 - (3 - 2\sqrt{2})^{2k-1} \right] (3 + 2\sqrt{2})^{n+1} \right. \\
& - \left[\sqrt{2} + 1 + (3 + 2\sqrt{2})^{2k-1} \right] (3 - 2\sqrt{2})^{n+1} \Big) \\
& \times \left(\left[1 - (3 - 2\sqrt{2})^{2k-1} \right] (3 + 2\sqrt{2})^{n+1} \right. \\
& + \left[1 + (3 + 2\sqrt{2})^{2k-1} \right] (3 - 2\sqrt{2})^{n+1} \Big)^{-1}. \quad (18)
\end{aligned}$$

Proof. By Lemma 7, we only need to compute the global cyclicity index of L_n . On one hand, by (9) in Theorem 6, for $1 \leq k \leq n$, we have

$$\begin{aligned}
\sigma_{L_n}(a_k, b_k) - 1 &= \sigma_{L_n}(b_k, a_{k+1}) - 1 \\
&= \sigma_{L_n}(a'_k, b'_k) - 1 = \sigma_{L_n}(b'_k, a'_{k+1}) - 1 \\
&= \left((3 + 2\sqrt{2})^{n+1} - (3 - 2\sqrt{2})^{n+1} \right)
\end{aligned}$$

$$\begin{aligned}
& \times \left(\left[1 - \frac{\sqrt{2}}{8} + \frac{\sqrt{2}}{8}(3 - 2\sqrt{2})^{2k} \right] (3 + 2\sqrt{2})^{n+1} \right. \\
& - \left[1 + \frac{\sqrt{2}}{8} - \frac{\sqrt{2}}{8}(3 + 2\sqrt{2})^{2k} \right] (3 - 2\sqrt{2})^{n+1} \Big)^{-1} - 1 \\
& = \left(\left[1 - (3 - 2\sqrt{2})^{2k} \right] (3 + 2\sqrt{2})^{n+1} \right. \\
& + \left[1 + (3 + 2\sqrt{2})^{2k} \right] (3 - 2\sqrt{2})^{n+1} \Big) \\
& \times \left(\left[4\sqrt{2} - 1 + (3 - 2\sqrt{2})^{2k} \right] (3 + 2\sqrt{2})^{n+1} \right. \\
& - \left[4\sqrt{2} + 1 - (3 + 2\sqrt{2})^{2k} \right] (3 - 2\sqrt{2})^{n+1} \Big)^{-1}. \quad (19)
\end{aligned}$$

On the other hand, by (10), for $1 \leq k \leq n + 1$, we have

$$\begin{aligned}
\sigma_{L_n}(a_k, a'_k) - 1 &= \left(\sqrt{2} \left[(3 + 2\sqrt{2})^{n+1} - (3 - 2\sqrt{2})^{n+1} \right] \right) \\
& \times \left(\left[1 + (3 - 2\sqrt{2})^{2k-1} \right] (3 + 2\sqrt{2})^{n+1} \right. \\
& + \left[1 + (3 + 2\sqrt{2})^{2k-1} \right] (3 - 2\sqrt{2})^{n+1} \Big)^{-1} - 1 \\
& = \left(\left[\sqrt{2} - 1 - (3 - 2\sqrt{2})^{2k-1} \right] (3 + 2\sqrt{2})^{n+1} \right. \\
& - \left[\sqrt{2} + 1 + (3 + 2\sqrt{2})^{2k-1} \right] (3 - 2\sqrt{2})^{n+1} \Big) \\
& \times \left(\left[1 - (3 - 2\sqrt{2})^{2k-1} \right] (3 + 2\sqrt{2})^{n+1} \right. \\
& + \left[1 + (3 + 2\sqrt{2})^{2k-1} \right] (3 - 2\sqrt{2})^{n+1} \Big)^{-1}. \quad (20)
\end{aligned}$$

By the definition of the global cyclicity index, it follows that

$$\begin{aligned}
 C(G) &= \sum_{k=1}^n [\sigma_{L_n}(a_k, b_k) - 1 + \sigma_{L_n}(b_k, a_{k+1}) \\
 &\quad - 1 + \sigma_{L_n}(a'_k, b'_k) - 1 + \sigma_{L_n}(b'_k, a'_{k+1}) - 1] \\
 &\quad + \sum_{k=1}^{n+1} [\sigma_{L_n}(a_k, a'_k) - 1] \\
 &= 4 \sum_{k=1}^n [\sigma_{L_n}(a_k, b_k) - 1] + \sum_{k=1}^{n+1} [\sigma_{L_n}(a_k, a'_k) - 1].
 \end{aligned}
 \tag{21}$$

Then (18) could be obtained by substituting (19) and (20) into (21). $\square$

As numerical results, global cyclicity indices of benzenoid chains from H_1 to H_{50} are listed in Table 1.

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